**6. Other features**

***6.1 Calculate RMSD***

This module is used to calculate RMSD between different poses of a ligand. RMSD is often used to measure the difference between two poses, which indirectly reflects the accuracy of docking results. Unlike the RMSD in the docking log file, this module allows you to calculate RMSD between any ligand poses and to set your own reference pose. It’s useful for comparing the co-crystal pose and re-docking pose, or the docking results from different docking software.

RMSD is calculated according to Trott et al (*Trott O., Olson A. J. J Comput Chem, 2010, 31(2): 455-461.*) in this module.

1. Click “Set the reference pose” to set which pose (.pdbqt) will be used as reference.
2. Click “Choose other poses directory” to set where other poses (.pdbqt) of the ligand are located. **Note that all the files in pdbqt format in this directory will be considered as the poses for RMSD calculation. The output of Vina cannot be used directly for the calculation, please split it first in module 5.2. Only the different poses of a ligand can be used for RMSD calculation, this module is not suitable for calculating RMSD between different ligands.**
3. Click “Choose saving directory” to set where the RMSD calculation results will be saved.
4. Click “Begin to calculate” and wait. When the calculation is complete, click “View results” to view the RMSD calculation results.

***6.2 Two ligands docking***

This function is a new feature in Vina 1.2.0. It can be used in the situations where two ligands interact with the receptor at the same time, such as substrate+cofactor+enzyme, inhibitor+substrate+enzyme, inhibitor+cofactor+enzyme, etc.

1. Click “Select ligand 1” and “Select ligand 2” to select two prepared ligands (.pdbqt).
2. Click “Select docking receptor” to select the prepared protein receptor (.pdbqt).
3. Click “Select config file” to select the config file containing the necessary docking parameters.
4. Click “Choose saving directory” to set where the docking results will be saved.
5. Click “Begin docking” and wait……The affinity score and docking poses can be found in the saving directory when the docking is complete.

**This module does not support batch docking. We strongly recommend that the docking box size should be as small as possible in the multi-ligand docking. The blind docking method is not acceptable, otherwise the ligands may be far apart after docking, which is of no research value**.

***6.3 Flexible docking (Induced fit docking)***

Flexible docking means that the conformations of both the key residues in the binding site and the ligand molecule can be changed to achieve an optimal binding state during the docking process (by default, Vina uses the rigid receptor docking method, i.e. only the conformation of the ligand molecule can be changed to fit its receptor). Flexible docking is designed to analyze more detailed interactions between the ligand and the receptor, which is also more in line with the actual binding process of biomolecules.

1. Click “Select a ligand” to select a prepared ligand (.pdbqt).
2. Click “Select a receptor” to select a prepared protein receptor (.pdbqt).
3. Click “Choose saving directory” to set where the docking results will be saved.
4. Return to module 1.2 to set the MGLTools installation directory.
5. Enter flexible residues. It is recommended to select 2~5 residues in the binding site that may significantly interact with the ligand.

If there is only one chain in the protein, the following simple format is accepted:

e.g. ARG405\_ILE84

Use “\_” to separate different residues.

If there is more than one chain in the protein, please enter the residues as follows:

e.g. hsg1:A:ARG8\_ILE84,hsg1:B:THR4

Name of the receptor, *colon*, capital letter of the chain in which the key residues are located, *colon*, abbreviation of a residue, index of the residue, *underscore*, the abbreviation of the next residue, index of the next residue, …, *comma*, capital letter of the chain in which the key residues are located, *colon*, the abbreviation of a residue, index of the residue, *underscore*, the abbreviation of the next residue, index of the next residue, …

**Note that the index of the residue should be less than 1000**.

This step will split the original *pdbqt* file into two parts, rigid receptor (\_rigid.pdbqt) and flexible residues (\_flex.pdbqt), which will be saved in the folder where the original receptor is located. The config file will be also generated automatically and saved in the saving directory.

1. Click “Begin docking” and wait……The affinity score and docking poses can be found in the saving directory when the docking is complete.

**This module does not support batch docking.**

**6. 其他功能**

***6.1 计算RMSD***

该模块用于计算同一分子不同构象间的RMSD。RMSD通常被用来衡量两个构象间的差异大小，间接反映了对接结果的准确性。与对接日志文件中的RMSD不同，该模块允许用户计算任意构象间的RMSD，并由用户指定参考构象。这对于比较共晶配体和重对接的结果构象，或不同对接软件对接结果间的差异很有用。

本模块中的RMSD是根据Trott等人的方法计算的 (*Trott O., Olson A. J. J Comput Chem, 2010, 31(2): 455-461.*)。

(1) 点击"选择参考构象"来设置哪个构象(.pdbqt)将被用作计算RMSD的参考。

(2) 点击"选择其它构象所在路径"来设置该分子其它构象(.pdbqt)所在位置。**请注意，该目录下所有*pdbqt*格式的文件都将被视为要计算RMSD的构象。Vina的输出不能直接用于计算RMSD，请先在模块5.2中分割为单独的构象。只有同一分子的不同构象可以用于RMSD计算，本模块不适合计算不同分子之间的RMSD。**

(3) 点击"选择保存路径"来设置RMSD计算结果的保存位置。

(4) 点击"开始计算"并等待。当计算完成后，点击"查看结果"即可。

***6.2 双配体对接***

该功能是Vina 1.2.0的新功能，可用于两个配体同时与受体发生作用的情况，如底物+辅因子+酶、抑制剂+底物+酶、抑制剂+辅因子+酶等的对接。

(1) 点击"选择一个配体"和"选择另一个配体"来选择要对接的两个配体(.pdbqt)，不分主次。

(2) 点击"选择对接受体"来选择一个准备好的蛋白质受体(.pdbqt)。

(3) 点击"选择配置文件"来选择包含必要对接参数的配置文件。

(4) 点击"选择保存路径"来设置对接结果的保存位置。

(5) 点击"开始对接"并等待，当对接完成后可以在保存路径中找到结合亲和力打分和对接结果构象。

**本模块不支持批量对接。我们强烈建议在多配体对接中，使用应尽可能小的对接盒子。盲对接是不可接受的，否则对接后配体间相隔甚远，无实际研究价值**。

***6.3 柔性对接(诱导契合对接)***

柔性对接是指在对接过程中，结合位点的关键残基和配体分子构象都可以自由改变，以达到二者最佳的结合状态(默认情况下，Vina使用半柔性对接方法，即只改变配体分子的构象来适应受体结构)。柔性对接是为了分析配体和受体之间更详细的相互作用，同时这也更符合生物分子的实际结合过程。

(1) 点击"选择一个配体"来选择一个准备好的配体(.pdbqt)。

(2) 点击"选择一个受体"来选择一个准备好的蛋白质受体(.pdbqt)。

(3) 点击"选择保存路径"来设置对接结果的保存位置。

(4) 返回模块1.2，设置MGLTools的安装路径。

(5) 输入柔性残基。建议在结合位点选择2~5个与配体有潜在相互作用的残基。

如果蛋白质中只有一条链，下面简单的输入格式是可接受的：

例如：ARG405\_ILE84

用"\_"来分隔不同的残基。

如果蛋白质中的链不止一条，请按以下方式输入柔性残基：

例如：hsg1:A:ARG8\_ILE84,hsg1:B:THR4

受体名称，*冒号*，关键残基所在链的大写字母，*冒号*，残基缩写，残基序号，*下划线*，下一个残基的缩写，下一个残基的序号，...，*逗号*，关键残基所在链的大写字母，*冒号*，残基缩写，残基序号，*下划线*，下一个残基的缩写，下一个残基的序号，...

**注意，残基的序号应该小于1000。**

这一步将把原始*pdbqt*文件分成两部分，刚性受体（\_rigid.pdbqt）和柔性残基（\_flex.pdbqt），它们将被保存在原始受体所在的文件夹中。配置文件也将自动生成并保存在结果路径中。

(6) 点击"开始对接"并等待，对接完成后可以在结果路径中找到结合亲和力打分和对接构象。

**此模块不支持批量对接**。